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Plastic Deformation in ODS Ferritic Alloys: A 3D Dislocation Dynamics Investigation

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Abstract

Discrete dislocation dynamics simulations were carried out to examine mechanical behavior of ferritic steel strengthened with Oxide Dispersion Strengthening (ODS) particles. Interplay of irradiation induced defect clusters and the ODS precipitates and its effect on the strain localization and hardening of the material is investigated. These simulations show that, in the absence of irradiation, the ODS particles act as an impediment to the dislocation motion and hence lead to greater strain localization, when subjected to uni-axial tensile deformation. After irradiation, however, it is seen that the presence of interstitial loops in the material reverses this trend. That is, presence of particles act against the detrimental effect of irradiation induced defect microstructure and helps in reducing strain localization. The hardening behavior also exhibits the same trend. Our study indicates that the irradiation induced hardening is suppressed by the presence of strengthening particles.

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Key words: ODS steels, dislocation dynamics, precipitate hardening, neutron-irradiation, ductility, cross-slip.

1. Introduction

ODS strengthened Ferritic steels are now considered to be prime candidates for nuclear applications involving high temperatures and irradiation doses. Inspite of a flurry of theoretical and experimental activity in these systems, understanding of the role of ODS precipitates in enhancing the mechanical behavior of the structual materials is far from complete. For example, It is found that certain ODS alloys exhibit better post-irradiation ductility and hardening characteristics in comparision with their single phase counterparts [1--5]. So far these beneficial effects are only partly explained in terms of their of dislocation mechanisms [6].

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In this work we examine, using discrete dislocation dynamics simulations, the role of impenentrable ODS precipitates in influencing the dislocation mobility and hence their impact on strain localization. Mobility rules used in evolving the dislocations in these simulations are based on thermal activation theory [7-8]. Implemented cross-slip behavior is based on recent investigation results on ferritic systems [9], including molecular dynamics simulations [10]. Our model hence includes the contribution of work hardening resulting from Orowan loops, as well as other factors, such as forest dislocation hardening. Irradiation effects are also examined, by introducing defect clusters in the form of dislocation loops, a feature common to a wide range of irradiation doses and temperatures, in metallic materials.

2. Simulation Details

The DD code used in this study is based on a discrete edge-screw model adapted to bcc crystalline structure, accounting for the twelve a/2{110}<111> slip systems. Velocity of edge segments is proportional to the effective resolved shear stress whereas the velocity of screw segments is taken to be proportional to $\exp(\Delta G/k_B T)$, where ΔG is the activation energy barrier to move a screw dislocation at a given temperature T. Cross-slip mechanism is treated according to a specific procedure, where the glide plane of each screw segment is updated at each time step, according to its physical selection probability. The latter quantities depend on the (updated) activation barriers associated to each possible glide plane. All details relative to the adopted cross-slip algorithm can be found in reference [11].

Irradiation loops formed at high temperature in Fe based bcc alloys are sessile (immobile), due to their specific Burgers vector [12-13]. Micro level simulations, involving one dislocation segment and six irradiation loops, have been performed to study the interaction of an incoming dislocation segment with these interstitial loops.

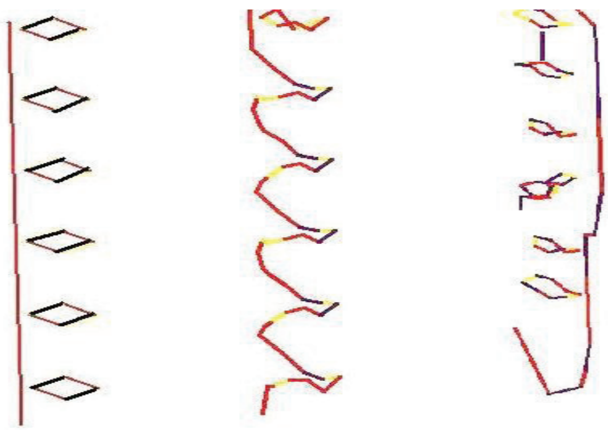
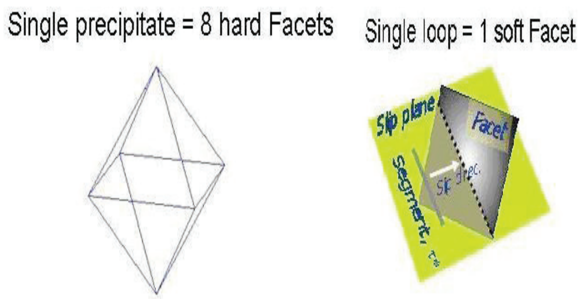


Fig 1: Micro level simulations of interaction of an edge dislocation with six interstitial loops.

It is found that the beyond certain resolved shear stress, the dislocation segment sweep through the irradiation loops leaving them behind. This behaviour is identical in both screw and edge cases except that the resolved shear stress for shearing through an interstitial loop is different for edge and screw dislocations. This behaviour is also seen in molecular dynamics simulations [14-15]. This feature of the interstitial loops allows them to be modelled as a single facet, instead of collections of dislocations. This will give a significant speedup in the computationa. However, unlike for precipitate-facets, facets describing irradiation-induced loops can be crossed by mobile dislocations: loop-facets are softer obstacles than precipitate-facets.



The ODS precipitates are regularly spaced in the form of a three-dimensional array. This arrangement allows for obtaining the maximal effect of particles, since strain localization in lower particle regions is avoided (finger path effect). Image forces due to the precipitates are also neglected, with a view to reduce the overall computational load as they are shown to have a limited influence on yield stress (less than +4%) and strain hardening characteristics of the crystal (less than +10%), especially when cross-slip is accounted for. [16].

3. Simulated cases

The DD simulations are performed in fixed plastic strain rate conditions, at room temperature (300°K). Four different cases are investigated, for analysis and comparison purposes:

- **Case-1:** Ferritic matrix (without hard particles and soft facets).
- **Case-2:** Mono-modal distribution of 0.5% volume fraction of hard r_p = 20 nm particles. The selected volume fraction is typical of recently developed ODS alloys.
- **Case-3:** Mono-modal distribution of 10^{20} m^2 density of soft 20 nm facets. Selected facet characteristics are corresponding to irradiation loops forming at intermediate temperature and dose ranges in pure Fe grains.
- **Case-4:** a bi-modal distribution including a 10^{20} m^2 density of soft D = 20 nm loop-facets and a 0.5% volume fraction of hard D = 20 nm particles. This configuration is consistent with 0.75 dpa irradiations performed at 400°C, in ferritic ODS system having similar characteristics as taken here (0.5% volume fraction of 28 ± 8 nm Y_2O_3 particles). This case applies to irradiated ODS alloys.

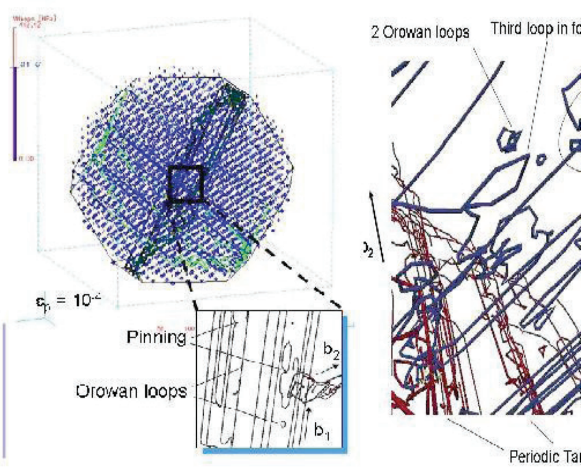


Fig 2 DD simulations results: the irradiated ODS grain case after cumulated plastic strain

All simulated grains are loaded in uni-axial tension along the (001) axis and initially, contain 2 edge dislocation sources (500 nm long). One source belong to the a/2(101) $[\bar{1}\,\bar{1}1]$ slip system, taken as the primary slip system; one source belongs to the a/2($\bar{1}$ 0 1)[$\bar{1}$ 1 $\bar{1}$] slip system, taken as the secondary slip system. The loading direction is highly symmetrical, since all slip systems are loaded with the

nearly same resolved shear stress (Schmidt factor is 0.41), a condition that also maximizes the time-dependent probability of cross-slip.
One of the configurations, matrix with ODS precipitates and dislocation loops is shown in Fig. 2 for illustration purposes.

4. Results and Discussion

When the applied loading is switched on, familiar slip characteristics of bcc systems, like random cross-slip, pencil glide, edge-screw mobility anisotropy and tension-compression anisotropy [7] are noticed in all the four cases. In simulations corresponding to case-1, in the stress-strain curve, a transient, high stress regime is first achieved. This regime corresponds to activation of the initial sources, where shear loops develop until stopped by the grain boundaries. New sources are then generated, initially by wandering mechanism involving cross-kinks and later on, by double cross-slip mechanism [17]. And hence the screw dislocation velocities are seen to stabilize to lower values as shown in the fig 3, where each point corresponds to one dislocation segment, at a given time step. The largest variations are observed during evolutions from transient to steady state. None of theses processes are imposed and emerge as a natural outcome of the simulations.

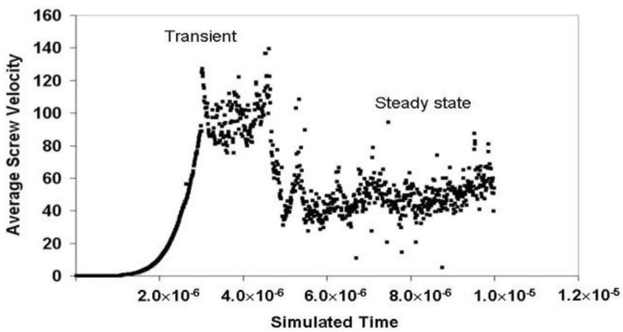


Fig 3.Analysis of average dislocation velocity evolution in the un-irradiated grain case.

While it is clearly beyond the scope of this paper to predict the experimental ductility loss of actual specimens, trends can nevertheless be examined quantitatively, at the scale of individual grains, as explained in Fig. 4.

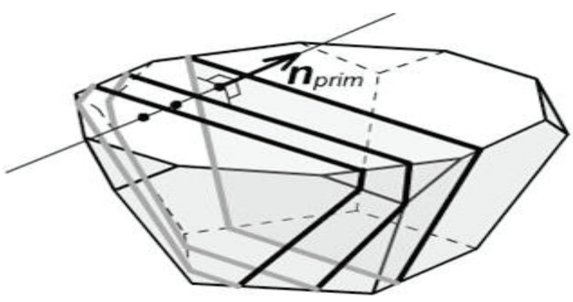


Fig 4.Analysis method for plastic strain spreading assessment (see also the main text).

Simulation volumes are first divided into N parallel sub-regions, parallel to primary slip plane, as shown in fig 4. The i^{th} region is considered as being active if dislocation density is non-vanishing there Spatial coordinate of the i^{th} plane region, x_i (in nm), is the distance of the plane i taken from a reference grain boundary along a reference axis normal to slip planes. The reference axis is divided into finite spatial intervals Δx ~ 10 nm, and results are displayed in the form of frequency versus position histograms. Broader distribution is considered as beneficial for residual ductility.

These distribution analysis was carried out in all the four simulations at a plastic strain level of $\varepsilon_p = 10^{-3}$. The initial dislocation sources are placed at the same locations in all the simulations.

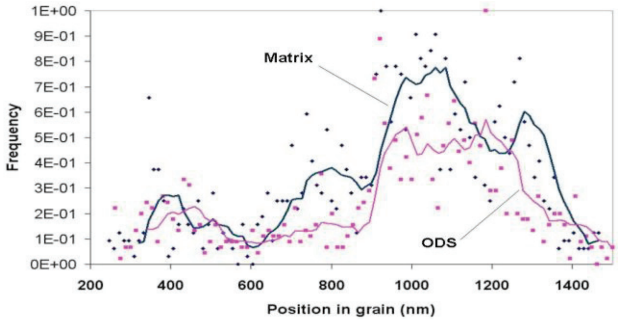


Fig 5.Dislocation density histogram for the matrix and precipitates cases computed at the same plastic strain level

The figure above illustrates that strain localization is more pronounced in ODS systems than pure ferritic grains. This result is consistent with experimental data obtained on ODS steels containing 20 nm particles, where uniform elongation is less than in its precipitate-free counterpart [2].

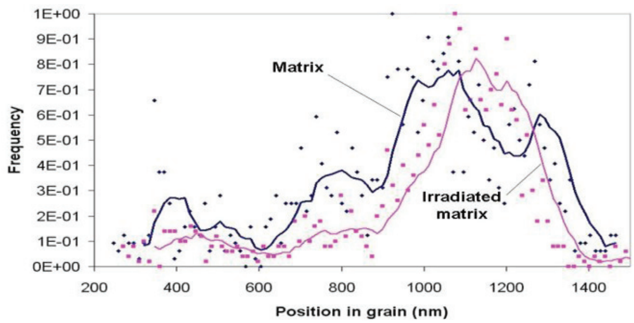


Fig 6.Dislocation density histogram for the un-irradiated matrix and the irradiated matrix

Comparing Fig 6 and Fig 7, it is obvious that after irradiation however, this trend is reversed. Namely, strain localization is more pronounced in irradiated matrix than in irradiated ODS grain. The model predictions are consistent with reported evidence that ODS alloys can be more resistant to post-irradiation loss of ductility than their non-ODS counterparts [1, 18].

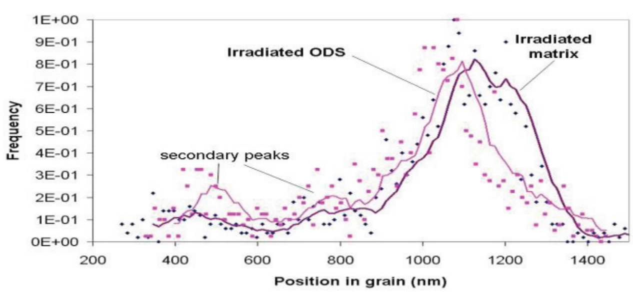


Fig 7: Dislocation density histogram for the irradiated matrix and the irradiated ODS

As a (beneficial) result, irradiation hardening due to defect loops is practically suppressed and plastic deformation spreading in the grain is much more homogeneous. Limited irradiation-induced hardening is also consistent with experimental data on similar ODS systems as investigated herein [19].

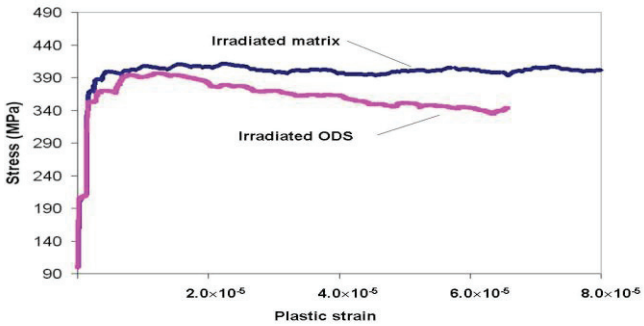


Fig 8: Stress-strain response of the case (4) and comparison with the same in non-irradiated ODS system, case (3)

5. Conclusion

Full three dimensional DD simulation of plastic deformation in 1 µm Fe grains have been performed, accounting for thermally activated glide and cross-slip of screw dislocations. Tensile load has been applied under multiple glide conditions, up to plastic strain of $\varepsilon_p = 10^{-3}$. Systematic comparisons between grains containing various types of internal obstacles have been presented, including: 20 nm hard ODS-like precipitates, 20 nm soft loop-facets and a bi-modal distribution of 20 nm ODS-like precipitates and loop-facets. Loop-facet strength introduced herein is as per MD simulation predictions of irradiation-induced dislocation loop defect clusters. DD simulation analysis show that, in absence loop-facets, ODS particles reduces dislocation mean free path and hence, lead to both material hardening and increased strain localization. In presence of irradiation-induced loop-facets however, simultaneous presence of particles reverses these trends. It that case namely, particles acts against the detrimental effect of irradiation-induced loops and helps in reducing strain localization. The same trend is obtained as regards irradiation-induced hardening, which is significantly diminished, by the ODS particles.

The present DD simulation work provides qualitative and quantitative insight regarding dislocation-based cause for beneficial effects of ODS precipitates. The available computational power however imposes limitations on the practical obstacle size used in this investigation. Hence, the minimum obstacle size corresponding to a fixed volume fraction of 0.5% is 20 nm. Experimentally, best material characteristics are obtained when using particle sizes well below 10 nm. Simulations corresponding to this situation imply a computational load about 1000 times as high as used herein. Work is now in progress to address difficulties associated with investigation of more advanced ODS systems.

References

[1] D.A. McClintock, M.A. Sokolov, D.T. Hoelzer, R.K. Nanstad, Journal of Nuclear Materials 392 (2009) 353-359.
[2] R. Schaeublin, T. Leguey, P. Spatig, N. Baluc, M. Victoria, Journal of Nuclear Materials 307-311 (2002) 778-782.
[3] A. Alamo, V. Lambard, X. Averty, M.H. Mathon, Journal of Nuclear Materials 329–333 (2004) 333-337
[4] N. Baluc, R. Schaublin, P. Spatig and M. Victoria, Nucl. Fusion 44 (2004) 56-61
[5] A. Ramar, N. Baluc, R. Schaublin, Journal of Nuclear Materials 367-370 (2007) 217-221.
[6] A. Kimura, H.S. Cho, N. Toda, R. Kasada, H. Kishimoto, N. Iwata, S. Ukai, S. Ohnuki, M. Fujiwara, Communication to Forschungszentrum Karlsruhe, Fortbildungszentrum (FTU), Germany, June 4-6, 2007.
[7] Caillard D, Martin JL. Thermally activated mechanisms in crystal plasticity. Oxford: Pergamon Press; 2003.
[8] D. Garcia, L. Dupuy, C. Robertson, M. Fivel, EFDA report, WP08-09-MAT-REMEV, Activity 4: Modeling mechanical properties, ET08-TTMS-006, 2008.
[9] C.F. Robertson, K. Obrtlik, B. Marini, Journal of Nuclear Materials, Vol. 366, pp. 58-69, 2007.
[10] Chaussidon J, Fivel M, Rodney D. Acta Mater 54 (2006) 3407.
[11] J. Chaussidon, C. Robertson, D. Rodney, M. Fivel, Acta Materialia 56 (2008) 5466-5476.
[12] M.L. Jenkins, Z. Yao, M. Hernandez-Mayoral, M.A. Kirk, Journal of Nuclear Materials 389 (2009) 197-202.
[23] J. Marian, B.D. Wirth, J.M. Perlado, Volume Physical Review Letters 88 (2002) 25.
[14] D. Terentyev, D.J. Bacon, Yu.N. Osetsky, Philosophical Magazine, (2009) 1-15
[15] D. Terentyev, P. Grammatikopoulos, D.J. Bacon, Yu. N. Osetsky, Acta Materialia 56 (2008) 5034-5046.
[16] C.S. Shin, M.C. Fivel and W W Kim, Modelling Simul. Mater. Sci. Eng. **13** (2005). 1163-1173
[17] C. Déprés, C.F. Robertson and M.C. Fivel, Phil. Mag. A **84** (2004) 2257
[18] M. Suzuki, A. Sato, N. Nagakawa, H. Shiraishi, Phil. Mag. A 65 (1992) 1309.

[19] H. Kishimoto, K. Yutani, R. Kasada, A. Kimura, Fusion Engineering and Design 81 (2006) 1045-1049.